CFD Evaluation of Sustainable Aviation Fuel Blends for Commercial Supersonic Technology

KUMUD AJMANI (HX5 LLC AT NASA GRC, CLEVELAND OH)
JEFFREY P. MODER (NASA GRC, CLEVELAND OH)

13TH US NATIONAL COMBUSTION MEETING
19-22 MARCH 2023, COLLEGE STATION, TEXAS
SUBTOPIC: ALTERNATE FUELS AND EMISSIONS -180AFE-0190

Motivation and Approach

- NASA's Commercial Supersonic Technology (CST) Project Goals:
  - Design a combustor that produces EINOx emissions in the 5-10 range at Supersonic Cruise conditions
    - CST Combustors will operate 'hot' for much longer durations (90-95% of cycle) than current subsonic combustors. Unique challenges for fuel burn, **emissions**, thermal stability of fuels and thermal load management.

- NASA Glenn Research Center's CST Project Focus (Combustion):
  - Evaluate emissions and performance of arbitrary blends of 'average' Jet-A (A2) and a sustainable fuel like GEVO Alcohol to Jet (C1), as compared to neat Jet-A fuel (baseline).

- Current Work: CFD analysis of RTRC/P&W Axially Controlled Stoichiometry (ACS) Combustor at supersonic cruise flight conditions using the Open National Combustion Code (OpenNCC)

Assess impacts of sustainable aviation fuel blends on combustor flame characteristics and gaseous emissions

Fuels: Jet-A, GEVO ATJ

- Average Jet-A (A2) evaluated as baseline fuel with OpenNCC for CST conditions
- GEVO ATJ (C1) chosen as sustainable fuel (1% aromatics, 99% *iso*-paraffins)
- DCN of C1 is much lower than that of A2. Fuel blends with relatively higher % of C1 potentially allow for greater mixing time, fewer local hotspots, better sustainability.

Nominal Composition	**Jet-A (A2)**	**ATJ (C1)**
aromatics	19%	1%
n-paraffins	20%	
cyclo-paraffins	32%	
iso-paraffins	29%	99%
Fuel Property		
Chemical Formula (Average)	$C_{11.4}H_{21.7}$	$C_{12.5}H_{27.1}$
H/C ratio	1.90	2.17
Derived Cetane Number (DCN)	47	16
Net heat of Combustion (MJ/kg)	42.8	43.9

Impact of arbitrary blending ratios of A2 with low-DCN C1 on flame, emissions

Liquid Fuel Properties for A2/C1 Blends

Liquid Property	Units	Average Jet-A (A2)	GEVO ATJ (C1)
Density	kg/m^3	1018.26 - 0.74617*T	967.01 - 0.72*T
Heat Capacity	J/kg-K	4.28*T + 723.0	4.10*T + 753.0
Viscosity	Pa-s	0.08949*exp(-0.01394*T)	1.89212*exp(-0.02393*T)
Vapor Pressure	Pa	10**(28.95 - 3000.4/T - 6.5*log(T) - 4e-4*T)	10**(28.9 - 3000.4/T - 6.5*log(T) - 4e-4*T)
Latent Heat	J/kg	3.8e5*[(Tc-T)/(Tc-298)]**0.375	3.6e5*[(Tc-T)/(Tc-298)]**0.375
Critical Temperature (Tc)	K	760.4	740.2

Liquid Transport Properties are assumed to be temperature dependent

Lucas Esclapez et. al *Combustion and Flame*, 181 (2017)

Liquid Fuel Property	A2	C1	% Diff C1 vs A2
Molecular Weight (g/g-mole)	**154.1**	**184.3**	**20%**
Normal Boiling Point (K)	**489.5**	**459.0**	**-6%**
Density at 1bar (kg/m^3)	**791.5**	**748.0**	**-6%**
Heat of Vaporization (kJ/kg)	**310**	**256.3**	**-17%**
Critical Temperature (K)	760.4	740.2	-3%
Critical Pressure (bar)	18.2	18.0	-1%
Critical Volume (cm^3/g-mole)	700.4	713.0	2%

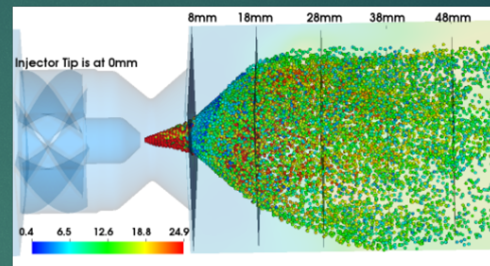
CFD implements temperature dependent liquid properties, multi-component spray and evaporation modeling for arbitrary blending ratios

Chemical Kinetics for OpenNCC

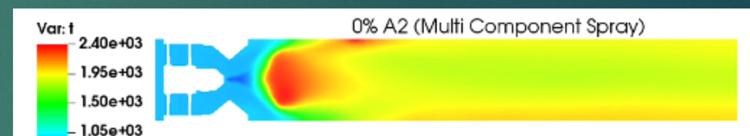
Kinetics Model	Jet-A (A2)	Gevo ATJ (C1)	A2/C1
Chemical Formula (Modeled)	$C_{11}H_{22}$	$C_{13}H_{28}$	$C_{11}H_{22}$ + $C_{13}H_{28}$
Number of Species	**41**	**42**	**51**
NOx Species	**30**	**24**	**30**
Source	HyChem [1]	HyChem [2]	HyChem [3]

[1] H. Wang et. al, *Combustion and Flame* 193 (2018) 502-519.
[2] K. Wang, et. al *Combustion and Flame* 198 (2018) 477–489.
[3] J-W. Park, et. al, https://web.stanford.edu/group/haiwanglab/HyChem/pages/download.html, 2019

Testing of HyChem A2/C1 Skeletal Kinetics with OpenNCC
Lean Direct Injector with Pressure Atomizer



Spray Particle Distribution
P_3=15atm, T_3=922K, ϕ=0.43



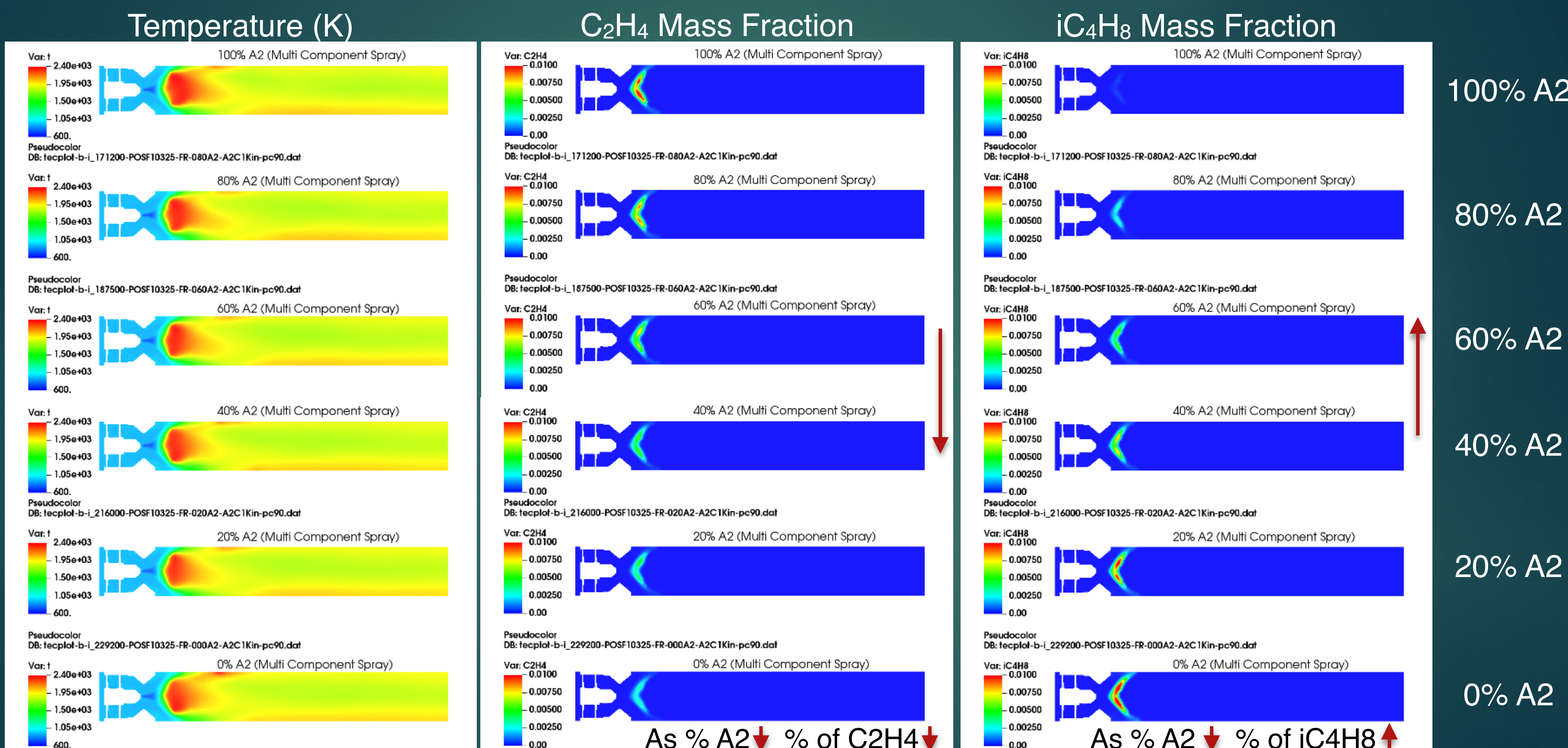
Lifted Flame in Axial Cross Section

Testing of HyChem A2/C1 Skeletal Kinetics with Cantera

Combustion Characteristic	100% A2	80% A2 20% C1	50% A2 50% C1	20% A2 80% C1	100% C1
Adiabatic Flame Temperature, K	1780.9	1781.5	1782.3	1782.9	1783.3
Ignition Delay Time, ms	24.9	21.4	18.6	19.1	22.4
Flame Speed, cm/s	32.6	32.1	31.7	30.8	30.2

Extensive validation of Kinetics and Multi-Component Spray Model for fuel blends

OpenNCC Testing for A2/C1 Kinetics

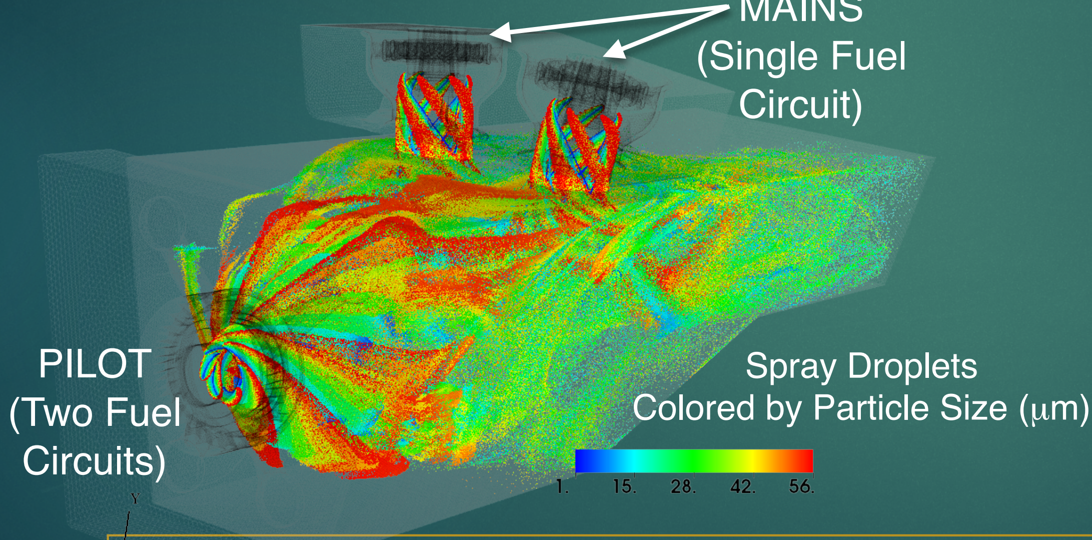


CFD trend of major pyrolysis species for A2 (C_2H_4) and C1 (iC_4H_8) matches measured data

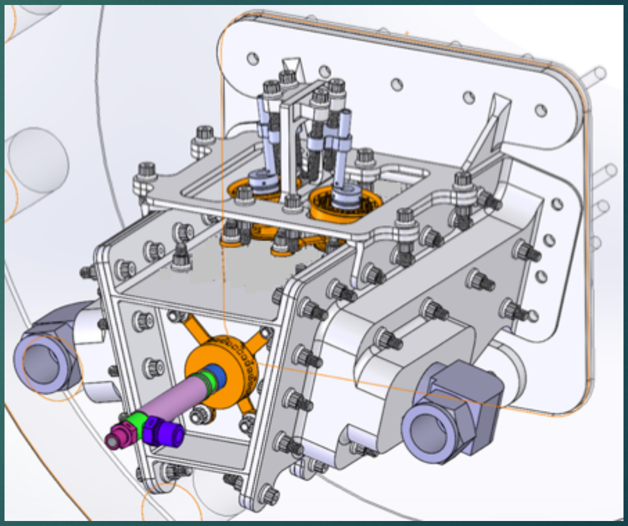
ACS Combustor CFD with OpenNCC

- RTRC/P&W Axially Controlled Stoichiometry (ACS) Combustor
- P_3=1.59MPa, T_3=884K, Dp = 3.5%, T_4=1780K (Experimental Condition, CST Cruise Point)
- Time-Filtered Navier Stokes, 4-stage Runge-Kutta with dual time-stepping, Finite rate kinetics, Lagrangian spray-modeling for multi-component fuel blends (80%, 50%, 20% A2)

ACS Combustor CFD Model

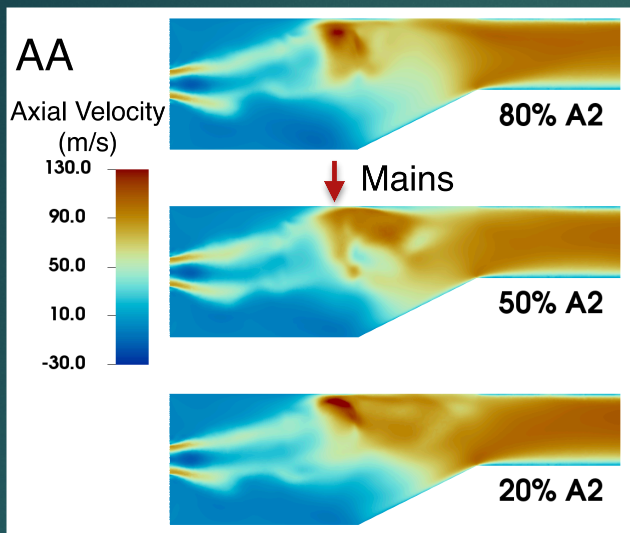


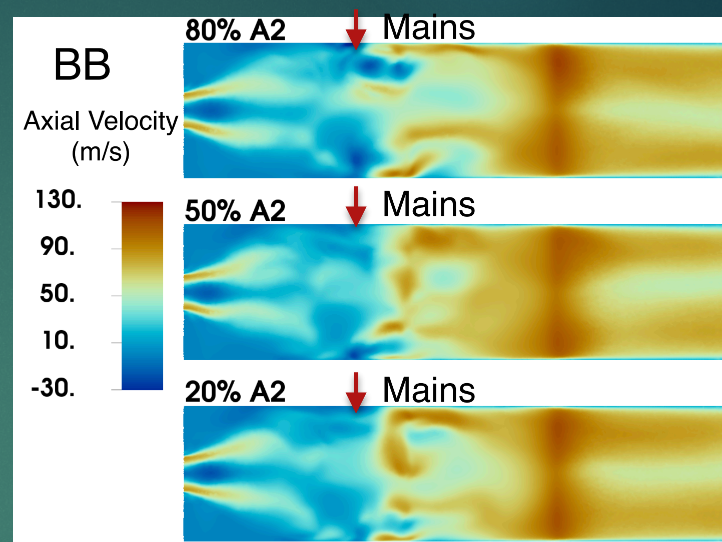
ACS Combustor Test Hardware

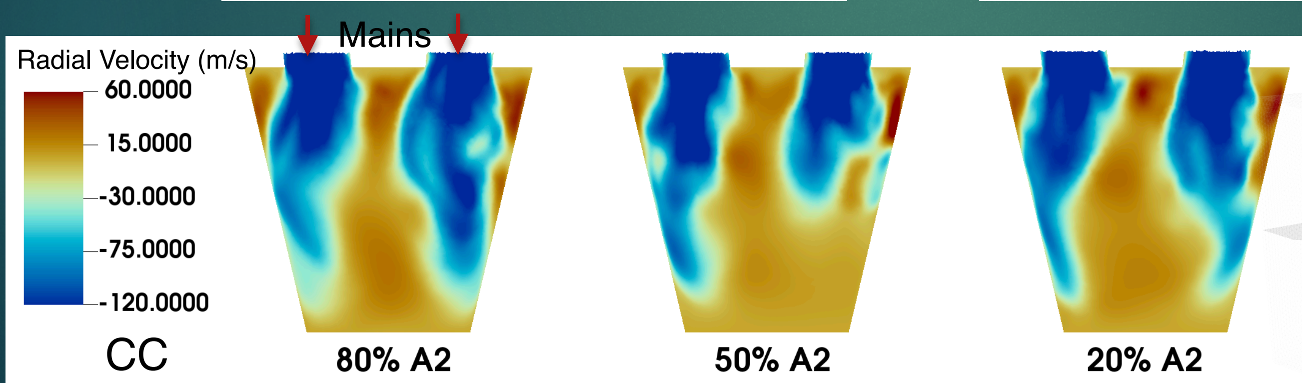


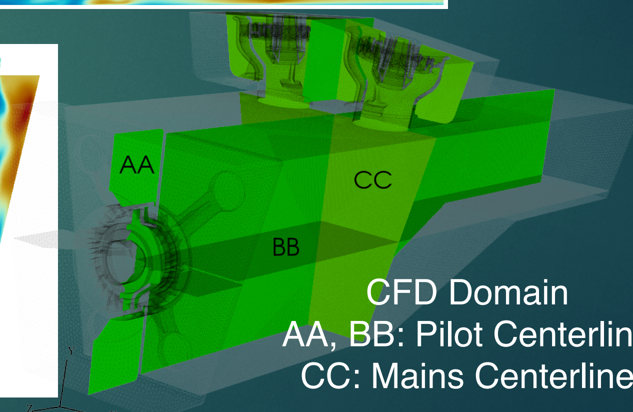
Two-Phase Reacting Flow CFD to predict flame-structure, emissions

Impact of A2 % on Aerodynamics



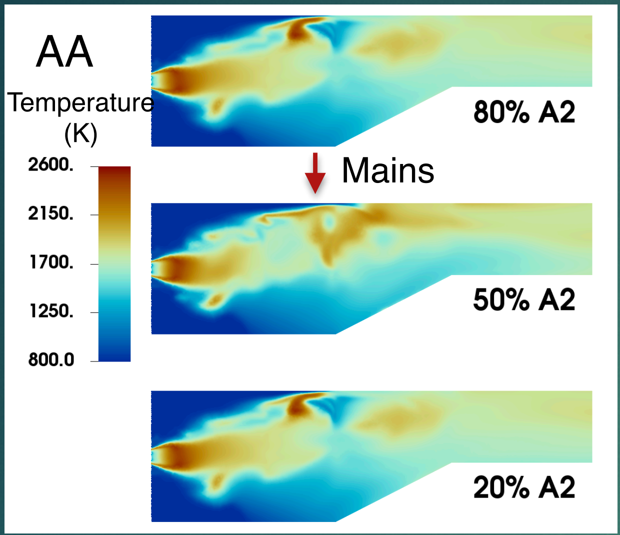


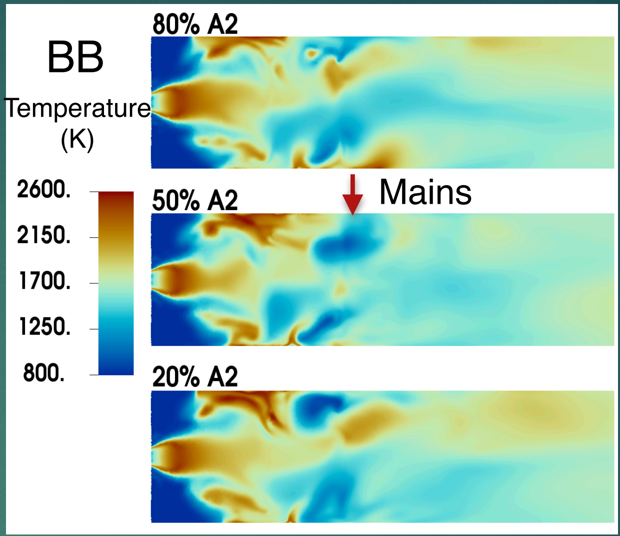


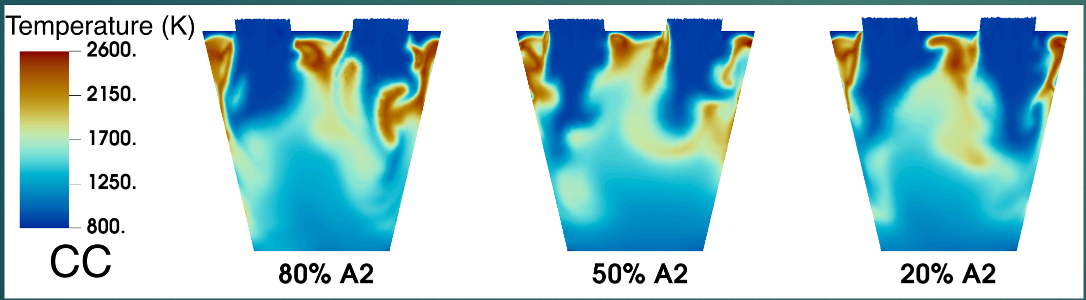


Similar reacting flow velocity profiles for Pilot and Main Injectors for all three blends

Impact of A2 % on Flame Structure





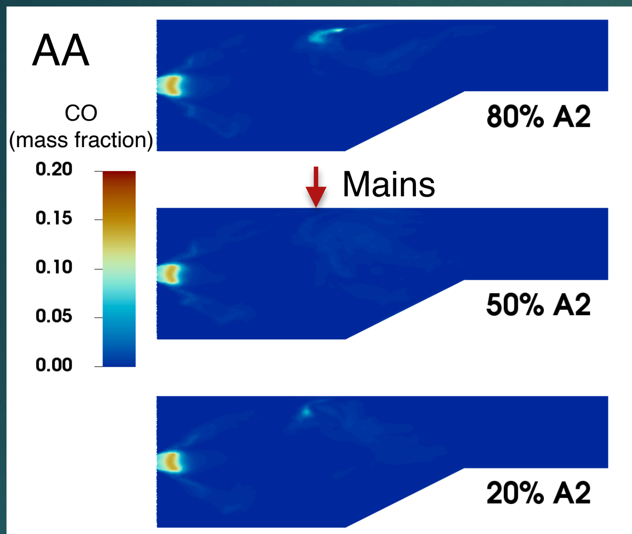


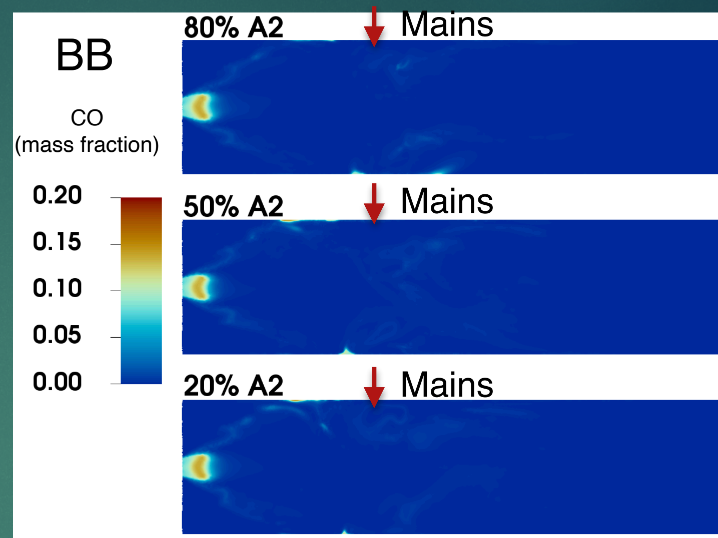
Experimental T4 for 100% A2 = 1781K

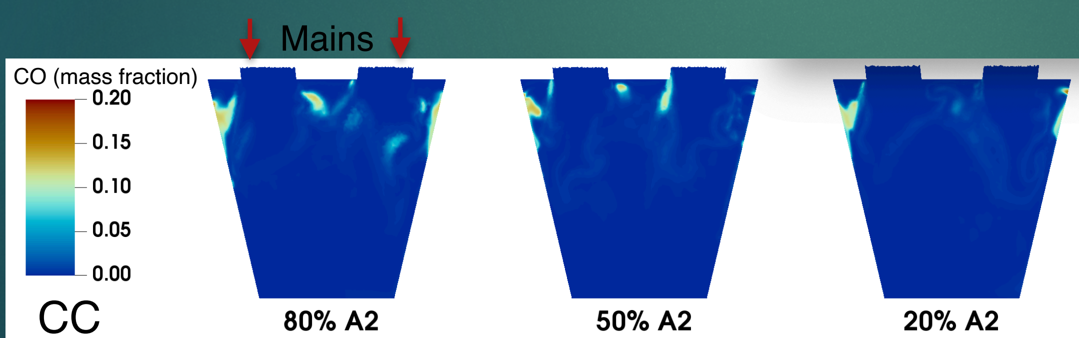
A2 %	CFD T4 (K) (Exit Plane Average)
100	1780
80	1785
50	1783
20	1780

Temperature profiles and flame structures for all blends are similar to each other

Impact of A2 % on CO Emissions





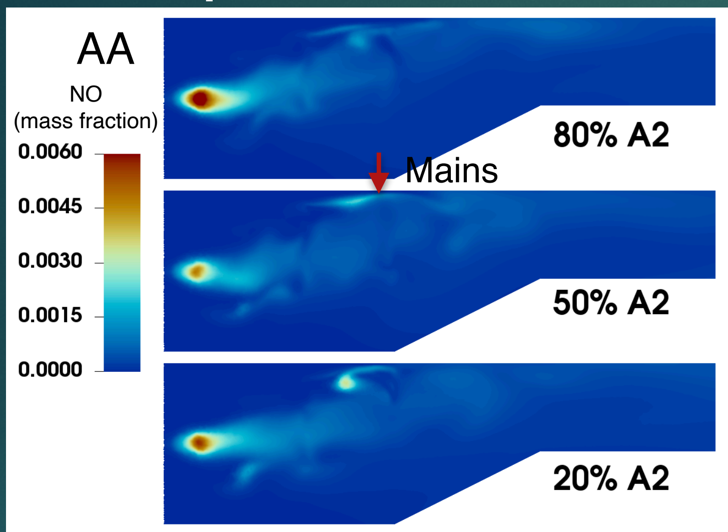


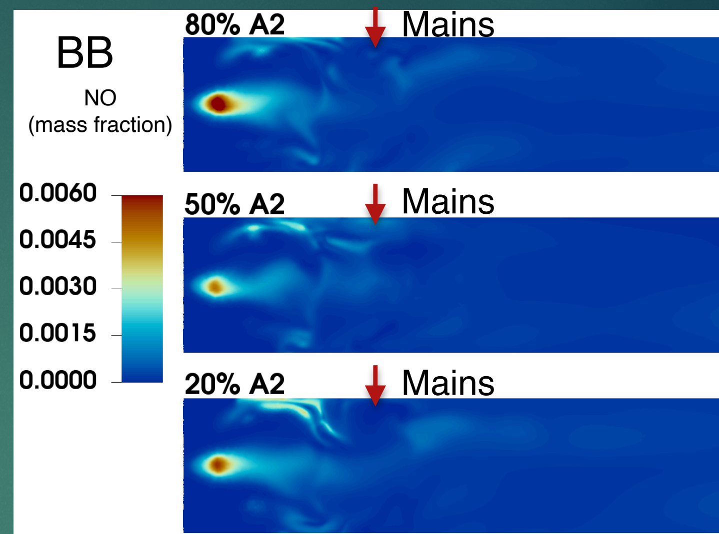
Experimental EICO for 100% A2 = 1.5

A2 %	CFD EICO (g CO/kg of fuel) (Exit Plane Average)
100	4.5
80	3.9
50	4.1
20	4.0

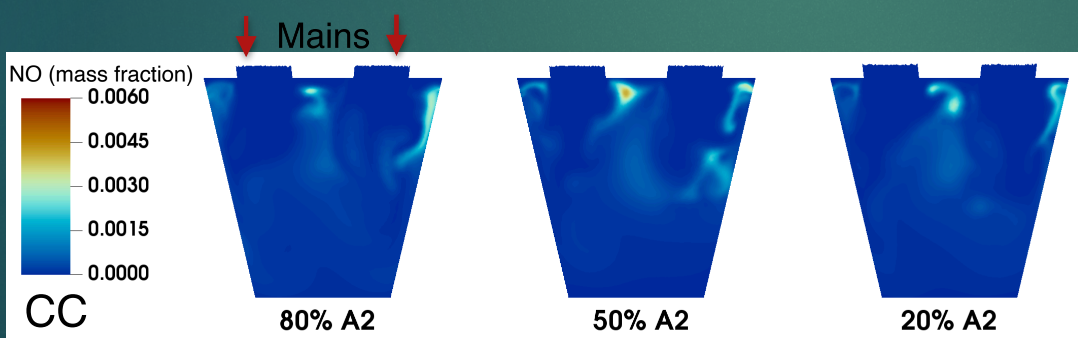
CFD: Majority of EICO produced by Main Injectors
Computed EICO values for all blends are within 15% of computed EICO for 100% A2

Impact of A2 % on NOx Emissions





Experimental EINOx for 100% A2 = 18 +/- 3.2



A2 %	CFD EINOx (g NOx/kg of fuel) (Exit Plane Average)
100	18.5
80	15.5
50	14.5
20	16.0

CFD: Majority of EINOx produced by Pilot Injectors
Computed EINOx values for all blends are ~15% lower than EINOx for 100% Jet-A

Summary and Significance

- The impacts of blending ‘average’ Jet-A (A2) and a sustainable aviation fuel, Gevo ATJ (Alcohol-to-Jet or C1) on flame structure and emissions at supersonic cruise conditions were successfully modeled with the OpenNCC code
- CFD results predicted only small variations in flame characteristics and NOx emissions for A2/C1 fuel blends ranging from 100% A2 to 20% A2/80% C1 burning in a next-generation axially-staged combustor operating at a supersonic-cruise stable-flame condition
- CFD predictions of EINOx for all fuel blends were within 10% of those for 100% Jet-A fuel, and within 10% of the lower end of the range of measured experimental values
- The current work demonstrated the capability to perform eddy-resolving CFD simulations including NOx chemistry for arbitrary fuel blends. The fuel blends studied captured a large range of variation in composition and combustion properties.

Acknowledgements

- This work was supported by the Commercial Supersonic Technology (CST) Project within NASA's Advanced Air Vehicles Program (AAVP), NASA Aeronautics Mission Directorate (ARMD)

- NASA Advanced Supercomputing (NAS) Facility at NASA Ames
- CUBIT mesh generation software (Sandia National Labs)
- VisIt flow visualization software (Lawrence Livermore National Labs)
- Lance Smith (RTRC): CAD for ACS Combustor Sector developed under NASA's Advanced Air Transport Technologies (AATT) Project